# Experimental report

20/02/2020

**Proposal:** 5-24-646 **Council:** 10/2019

**Title:** Peculiar structural transitions inUIrSi3

**Research area:** Physics

**This proposal is a new proposal**


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**Samples:** UIrSi3

| Instrument | Requested days | Allocated days | From | To |
|---|---|---|---|---|
| D1B | 2 | 1 | 06/02/2020 | 07/02/2020 |


## Abstract:

RTX3 compounds crystallizing in the non-centrosymmetric BaNiSn3-type structure reveal frequently diverse and exotic physical properties. UIrSi3 is one of the only two UTX3 isostructural analogs. A complex magnetic phase diagram and most probably a complex magnetic structure make UIrSi3 a prominent system for detailed microscopic investigations. Besides intensive investigations of macroscopic properties, we performed neutron diffraction experiments on single crystal employing CYCLOPS and D10 diffractometers. Except the information on magnetic structure of the compound, the obtained data showed a stable BaNiSn3-type structure down to low temperature. Surprisingly, our recent powder data from D7 experiment reveal a strong evolution of nuclear signal with temperature. A high temperature BaNiSn3-structure peaks remain in diffraction patterns down to 2 K, however a new set of peaks is revealed cooling the sample below 60 K. These peaks shift with further temperature decrease to higher angles and another set of peaks appears below 35 K. We propose an experiment employing D1B diffractometer to inspect these structural changes and their probable connection to magnetic order in detail.

## Peculiar structural transitions in $UIrSi_3$

The powder neutron diffraction experiment on $UIrSi_3$ sample was performed employing D1B diffractometer.

$UIrSi_3$ compound crystalizes in non-centrosymmetric tetragonal structure of $BaNiSn_3$-type. The compound is antiferromagnetic below $T_N = 41.7$ K. Application of magnetic field along tetragonal *c*-axis causes induced metamagnetic transition (MT); the critical field of $\mu_0 H_c = 7.3$ T at 2 K. The MT is first-order phase transition with asymmetric field hysteresis at temperature up to ~ 28 K. Above this so called tricritical point a second-order magnetic phase transition is identified [1, 2].

Recent neutron diffraction experiments on an $UIrSi_3$ single crystal on CYCLOPS and D10 diffractometers brought an evidence on both the nuclear structure and magnetic ordering of the compound. The refinement of nuclear structure based on 129 reflections (40 independent reflections) confirmed the non-centrosymmetric tetragonal structure of $BaNiSn_3$-type to be the crystal structure of $UIrSi_3$. Fullprof package's agreement factors were $R_B = 0.596\%$ and $R_F = 2.94\%$. No additional nuclear reflections were observed down to low temperature. Simultaneously, the antiferromagnetic ordering of U moments was revealed by a number of magnetic reflections outside of nuclear Bragg positions and described by a single propagation vector $\boldsymbol{k} = (0.1, 0.1, 0)$. The temperature evolution of magnetic and nuclear reflections was followed in temperature range from 1.7 K to 50 K. An integrated intensity of nuclear reflections remains the same (within the error) within whole investigated temperature interval revealing no magnetic intensity on nuclear reflections positions. The intensity on magnetic reflection positions remains constant up to ~20 K and decreases with increasing temperature. No magnetic intensity is observed at temperatures above $T_N$ well in agreement with macroscopic properties measurements.

Surprisingly, our recent diffuse scattering experiment on D7 diffractometer, primarily focused on signs of diffuse scattering around nuclear reflections, has brought new questions on nuclear and magnetic structure by observing new (nuclear) peaks below 60 K and 30 K. The structure stability/instability of the $UIrSi_3$ compound in powder form was the main question addressed to neutrons for experiment on D1B.

D1B experiment was performed with the wavelengths of 2.58 Å and 1.28 Å to investigate both magnetic and nuclear signal, respectively. The main focus was dedicated to the temperature range between 1.5 and 60.0 K to fully disclose the ambiguous behavior observed on D7 data. We note that the sample absorption (high neutron absorption cross-section of Ir) played significant role during the experiment. The diffraction patterns were measured with high statistics of approximately 5 hours/pattern, showing relatively weak nuclear peaks, and additional peaks from vanadium sample container, on high background. Taking into account the absorption and relatively small magnetic moments of U, we did not observe any difference between diffraction patterns measured at base temperature and in paramagnetic state. The antiferromagnetic order and propagation vector cannot be confirmed by our powder diffraction data. Diffraction patterns measured at several different temperatures revealed no other reflections except those expected for $BaNiSn_3$-type tetragonal structure (see in Fig.1 for 1.5 K). No signal was detected on positions of additional peaks observed during D7 experiment. As the same powder $UIrSi_3$ sample was used for both diffraction experiments (D7 and D1B), the structure instability and/or foreign phases in the powder sample has been excluded. Such

conclusion is of high importance for our single crystal data treatment, namely refinement of magnetic structure of $UIrSi_3$.

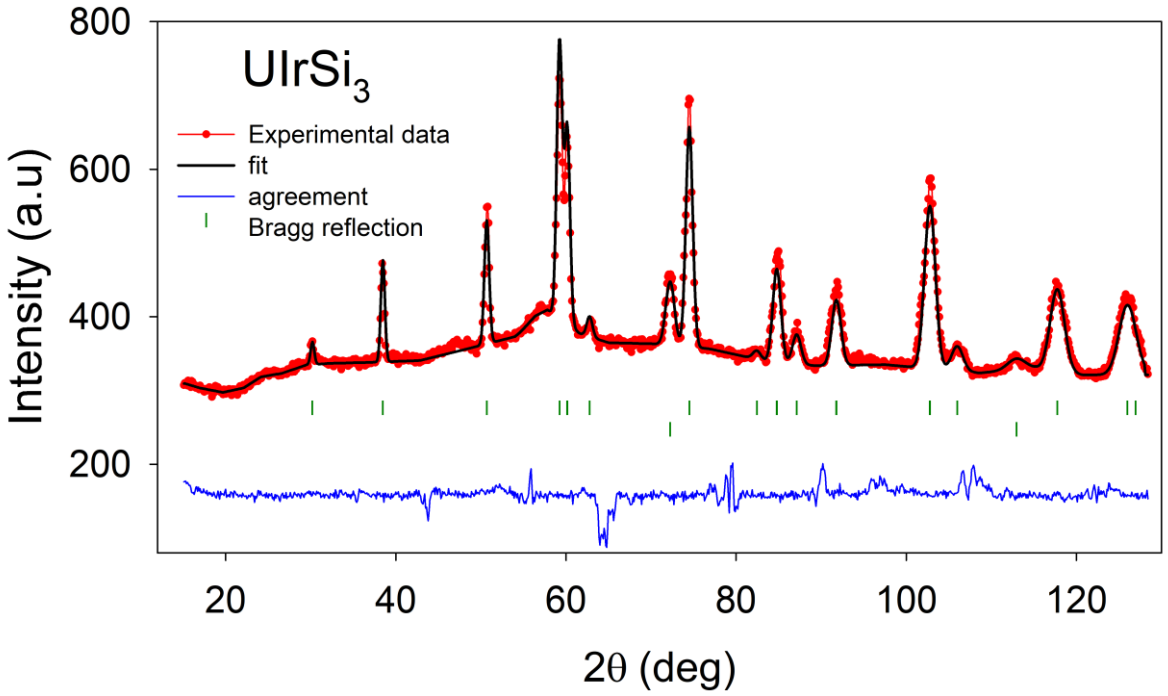


Fig. 1: Neutron diffraction pattern measured at 1.5 K on D1B for $UIrSi_3$ powder sample. The fit is performed for $BaNiSn_3$-type tetragonal structure and vanadium container.

The additional signal observed in course of D7 experiment has been identified as a possible presence of undesired gas in the aluminum sample container during diffraction experiment on D7. We have found that nitrogen dioxide possess two structures in solid state: hexagonal close packed structure with symmetry *P 63/m m c* between 63 K and 35 K; cubic structure described by space group *P a -3* below 35 K. These phases of $N_2$ agree qualitatively with additional reflections observed in D7 data.

[1] J. Valenta, F. Honda, et al., Phys. Rev. B 97, 144423 (2018).

[2] F. Honda, J. Valenta, et al., Phys. Rev. B 100, 014401 (2019).